



# Short Review of Studies on Modeling of Technology and Technical Means Used for Production of Classical and Nanomodified Functional Polymer Composite Materials

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## Abstract

The paper briefly announces the results of many years of research in the field of modeling and design of parameters of technology and technical means for production of classical and nanomodified functional polymer composite materials for structural purposes. Models of oriented structurally inhomogeneous media are considered which form the basis for designing parameters for technological methods of impregnation and winding, as well as for predicting the stress-strain state of classical polymer composite materials. Ultrasonic treatment is being investigated as a basic method of intensifying technological processes as well as improving the physico-mechanical and operational properties of classical and nanomodified functional polymer composites. The main parameters and features of the ultrasonic treatment modes are described. The results of modeling and designing of manufacturing technology parameters for production thermoplastics are presented. The aspects of the production technology for nanomodified functional polymer composite materials for functional purposes are provided.

**Keywords:** Modeling; Design; Technology; Composite; Nanomodification; Ultrasonic.

## 1. Introduction

Constructional polymer composite materials (PCM) are now widely used in various fields of industry: sports industry, medicine, aircraft building, automotive industry, construction and other industrial sectors.

The requirements imposed on construction functional materials used in load-bearing elements are high strength and rigidity, stability to dynamic loads, low mass, high durability, thermal and corrosion resistance and high reliability. Nanomodified (NM) PCM (NMPCM) fibrous reinforcing fillers (e.g., carbon fibers) and a polymer binder (PB) containing nanoparticles are intended primarily for use in high-load and especially reliable items.

At the same time, ultrasonic (US) treatment is the dominant method of physical modification for the production of classical and NM PCMs for functional purposes.

Methods of mathematical, structural-parametric and computer modeling are widely used to determine the parameters of technology and technical means for the production of classical and NM functional PCMs for structural purposes. Some studies in which significant results are obtained are briefly described below.

## 2. Modeling the Parameters of the Structure and Technologies for Obtaining Classical Reactoplastic Polymer Composite Materials

### 2.1. Structural Models of Oriented Structural-Non-Homogeneous Media

Models of structurally inhomogeneous media [1], applied to classical fibrous reactoplastic PCMs, allow to solve at least two problems at the same time. First, they allow to design the parameters of the basic technological operations (impregnation, winding, drying, etc.). Second, it becomes possible to predict the stress-strain of the produced composites. This allows to control the functional applicability of a composite obtained using a specific technology. Therefore, the determination of the parameters of such models is important.

The developed approaches to modeling the parameters of such models are described in the studies [2, 3].

### 3. Ultrasonic as the Dominant Method for Production of Classical and Nanomodified Polymer Composite Materials

#### 3.1. Production of Classical Polymer Composite Materials Using Ultrasonic

Ways for development of improved processes and production facilities for cavitation treatment that generate US vibrations required for specific processes, in particular by varying frequency, intensity, amplitude, time, temperature and pressure are important.

Problem situations for the basic production cycle of preparing reinforced objects of composite epoxy polymers (EPs) are considered in [7]. The expedience of using US modification in order to achieve energy saving and improve object quality is substantiated.

Known effective methods for treating liquid reactoplastic media (epoxy oligomers and epoxy compositions – ECs) using low-frequency US modification to improve their processing and operating properties are analyzed in [8]. Results of experimental studies are provided.

The effect of low-frequency US treatment regime and excess pressure on reactoplastic PCMs (unfilled and filled with short-fiber fillers) is studied in [9]. Optimum process parameters are established for US treatment of liquid ECs. The effect of low-frequency US treatment regimes on reactoplastic PCM operating properties is considered in [10]. An example is provided of effective US treatment by the technology developed compared with known methods.

The effect of heterofrequency US treatment on reactoplastic PCM operating properties is presented in [11]. Conformity is established for effective process parameters of heterofrequency US cavitation in liquid EPs, and this makes it possible to select effective energy saving processing base parameters for preparing EPs based upon them.

### 3.2. Intensification of the Impregnation Process and Strengthening of Composites

The main prerequisites for using US treatment for intensifying production of reactoplastic PCMs, in particular the main physical and chemical effects arising during pulsations of vapor and gas bubbles with cavitation action are analyzed in [12, 13]. Effect of parameters of US treatment on strength properties of epoxy binders and wound fibrous composites are investigated in [14].

Tests of annular PCM specimens – fiberglasses and organoplastics formed by the method of “wet” winding using low-frequency US – were conducted in [15]. Three alternate US-impregnation schemes were investigated. Optimal alternate schemes and insonification parameters were established experimentally: frequency, amplitude, intensity, and time. Optimization was carried out on the basis of investigation of the relationships between the values of the tensile, compressive, bending, and interlayer-shear strengths, and also the relative content of filler as a function of treatment parameters. It was shown that deviation of insonification parameters from the optimal leads to a reduction in strength characteristics, as well as to a different character of specimen failure in tension and interlayer shear.

## 4. Designing of Technical Tools Parameters for Obtaining of Classical Polymer Composite Materials Using Ultrasonic

An improved method has been developed to select efficient design and operating parameters for equipment used for the US modification of liquid-polymer composites and fibrous fillers [16]. The method can make US treatments more productive and speed up the processes of impregnation and batch-dosing in the molding of polymeric composites.

An approach for computer-aided design applying principles based on structural-parametric geometric modeling methodology for determining structural and technological parameters of technical ways to mold reactoplastic fiber PCMs using US treatment is developed in [17]. A general structural-parametric model is developed for a production process of composite fiber material preparation presented in the form of three consolidated blocks: epoxy resin US treatment and impregnated composite preparation; fiber material impregnation with PB; dosed application of PB into impregnated fiber material.

Analytical peculiarities of US cavitators based on piezoceramic transducers with a radiative plate, which experiences bending vibrations, are analyzed in [18]. The acoustic dimensions of components of a sectional piezoelectric transducer used in the production process of contact US treatment of a dry 1120-mm wide cloth impregnated with a PB, are calculated.

## 5. Modeling Parameters of Technology and Technical Means for Thermoplastics Molding

### 5.1. Manufacturing Technology of Thermoplastics: Modeling and Designing

Coordination of production-equipment output for manufacture of corrugated pipes is considered in [19]. Effects of volume change, the influence of subsequent stages in the shaping of a blank on the wall thickness of the latter and the productivity of the equipment are considered.

An approach to determination of geometric parameters of corrugated tubular articles, which makes it possible to relate structurally assigned parameters of the corrugation layout to the thickness of the product being extruded with the geometric profile dimensions of the corrugation being shaped, is proposed in [20]. Cases of free shaping of the arch of the corrugation, shaping of high-profile corrugations with inclined walls, and shaping of a low-profile corrugation are examined. Generalization is offered for any types of corrugated tubular articles.

A mathematical description of welding processes for layers of pipe is offered in [21]. Conditions for welding of the layers are formulated. Numerical solution of temperature distribution in the welding zone is described.

Results of analyses of the profile shaping of a corrugated pipe are presented in [22]. Cases of the shaping of a low-profile corrugation, and the shaping of a high-profile corrugation with vertical and inclined walls and a plane and circular arch are examined.

Non-isothermal mixing in the barrel mixer of an extruder by the method of numerical modeling is studied in [23]. The distribution of the travel speeds of the polymer melt that flows within the effective channels of the drum mixer under various temperature and deformation reworking conditions, as well as the structural characteristics of the mixer is established as a result of numerical investigations.

Use of a Phan-Thien-Tanner model for simulating viscoelastic liquid flow at the outlet from an extruder molding tool is proposed in [24]. A dependence for free extruded surface profile of cylindrical extruded objects on Deborah number is determined. Modeling results may be used for selecting extrusion processing regimes and in designing new extrusion heads with the aim of improving object quality characteristics.

Improved physical and mathematical models of polymer melting in screw extruder channels are presented in [25]. The basic distinction of these models is that three phases, namely, a solid porous plug, a mixture of melt, solid granule residuals, and gas, and a fully molten material, interact in the melting zone. Distributions of speed and temperature of the material in the screw channels are determined with due regard for the influence of barodiffusion, convection, and collapse of the plug. Evolution of plug collapse and melting processes is studied.

### 5.2. Connection and Repair of Polyethylene Pipelines Using Ultrasonic Modification and Heat Shrinkage

Aspects of the connection and restoration of polymeric pipelines for gas transport with the use of coupling and glue technologies based on heat-shrink couplings and glue compositions formed from EPs are analyzed in [26]. The effectiveness of epoxy glue compositions and the method for their US modification is substantiated. It is noted that effective US treatment makes it

possible to enhance deformation-strength and adhesion characteristics of the polymeric composites obtained, which can be used for the repair and restoration of polymeric pipelines, and to reduce the level of residual stress in these pipelines, and lengthen their service life.

Production bases developed for the molding of epoxy repair couplings with shape memory are described in [27]. It is established that maximum deformation of tubular blanks of the EPs under investigation, which had not been exposed to US vibrations, did not lead to their failure and amounted to no less than 15 – 17%. Variation in the strength of heat-shrinking couplings based on ECs is studied as a function of the parameters of their US treatment. Effective regime parameters for the US treatment, which contribute to maximum strain hardening of the couplings with retention of an acceptable degree of their deformation, are presented.

Effective surface-treatment methods for polyethylene pipes connected by banding with couplings and modeling tape impregnated with ECs are analyzed in [28]. The effectiveness of the method developed of complex US modification of the surface of polyethylene pipes, which leads to a 55 – 60% increase in in-service characteristics of the repair banded connection as compared with familiar methods, is substantiated.

The characteristics and sequence of practical implementation of production bases developed for the connection and repair of polyethylene pipelines using epoxy-glue compositions and banding are examined in [29]. The effectiveness of the complex US effect is substantiated in the production bases developed, and, to wit: when glue compositions are exposed to sonic vibrations, and during their impregnation with glass tape, as well as modification of the polyethylene pipes that are being connected.

Aspects of the use of effective hardware for thermistor couplings and components, which are used for thermistor welding in the repair of low- and medium-pressure polyethylene pipelines are investigated in [30]. Parameters of thermistor welding, and namely, the limiting values of the electric resistance, welding time, welding voltage, and the time required to cool the butt joints, are analyzed as a function of the diameter of the polyethylene pipelines and the type sizes of the connecting thermistor couplings or components.

## 6. Aspects of Production Technology for Nanomodified Polymer Composites on Functional Purpose

The prospects for development and practical application of nanotechnology, including for production of NMPCMs, in terms of the achievements of modern science and technology were provided in [31]. Characteristic features of nanofillers and possible future applications of carbon nanotubes (CNTs) were studied. The directions in which NMPCM's production technology is developing, including economic aspects of implementing their formation nanotechnologies, were described.

Effective patents protected technical means (methods and devices) designed to produce reactoplastic NMPCMs that provide increased strength and service life for structures based on them were considered in [32]. It was shown that technical means using low-frequency US cavitation were effective. This was due to the difficulty of providing a uniform distribution of nanoparticles in the oligomer because of the tendency of the added nanoparticles to attract each other and the resulting adhesion and aggregation.

Effective methods for dispersing CNTs in organic solvents and liquid polymeric media were analyzed in [33]. The relationship of these methods for improving the operational performance of NMPCMs was studied. It was shown that the conditions necessary to create such materials are a small size and a distribution of carbon nanofiller particles as uniform as possible in the liquid polymeric matrix. The tendency of the carbon nanofiller to

aggregate prevented the preparation of stable dispersions in water and organic solvents.

Features and problems of producing reactoplastic NMPCMs using modification of epoxide oligomers (EOs) with CNTs as an example were considered in [34]. Results from dispersion of highly viscous suspensions of EOs with CNTs by a rolling method and by induction of low-frequency US cavitation were discussed. The efficiency of introducing the nanoparticles into the liquid polymer medium depended on not only the dose but also the mixing parameters.

The characteristics of reactoplastic NMPCMs using structural carbon-fiber prepreps as examples were examined in [35]. The potential for application of structural carbon-fiber plastics in loadbearing elements was shown. A promising solution to the problem of surface modification of carbon-fiber plastics and PBs for improvement of the mechanical properties of the final product was to create a carbon-fiber-plastic combined filling in which a continuous carbon fiber was combined with a PB in which ultrafine carbon nanoparticles were uniformly distributed.

When sonicating liquids at high intensities, the US waves that propagate into the liquid media result in alternating high-pressure (compression) and low-pressure (rarefaction) cycles, with rates depending on the frequency of US. During the low-pressure cycle, high-intensity US waves create small vacuum bubbles or voids in the liquid [36]. When the bubbles attain a volume at which they can no longer absorb energy, they collapse violently during a high-pressure cycle. This phenomenon is termed US cavitation. During the implosion very high temperatures (approximately 5,000 K) and pressures (approx. 2,000 atm) are reached locally. The implosion of the cavitation bubble also results in liquid jets of up to 280 m/s velocity. The ultrasonically generated cavitation causes chemical and physical effects, which can be applied to processes.

Cavitation-induced sonochemistry provides a unique interaction between energy and matter, with hot spots inside the bubbles of ~ 5000 K, pressures of ~1000 bar, heating and cooling rates of  $> 10^{10}$  K/s. These extraordinary conditions permit access to a range of chemical reaction space normally not accessible, which allows for the synthesis of a wide variety of unusual nanostructured materials [36].

For example, since the extraordinary characteristics of graphite are known, several methods for its preparation have been developed. Beside to chemical production of graphenes from graphene oxide in multi-step processes, for which very strong oxidizing and reducing agents are needed. Additionally, the graphene prepared under these harsh chemical conditions often contain a large amount of defects even after reduction compared to graphenes obtained from other methods. However, US is a proven alternative to produce high quality graphene, also in large quantities [37].

Researchers have developed slightly different ways using US, but in general the graphene production is a simple one-step process. To give an example of a specific graphene production route. Thus, graphite is added in a mixture of dilute organic acid, alcohol, and water, and then the mixture is exposed to US irradiation [38]. The acid works as a "molecular wedge" which separates sheets of graphene from the parent graphite. By this simple process, a large quantity of undamaged, high-quality graphene dispersed in water is created.

## Conclusion

A wide range of issues in modeling and design of parameters of technology and technical means used for production of classical reactoplastics and thermoplastics as well as and NM functional PCMs are studied.

The effect of US modification in producing of the classical and NM functional PCM is provided by an increase in structural uniformity, US intensification of impregnation, and improvement of the strength and operational properties and production characteristics of the polymer matrix, as well as by a reduction in

the composite's effectiveness as a result of a reduction in the content of air inclusions and improvement of the binder's distribution across the section of the filler.

For the same reason, effective methods for facilitating aggregate disintegration, including use of low-frequency US during production of NMPCMs, are being actively pursued. Ways are indicated for development on this basis of improved processes and production facilities for cavitation treatment that generate US vibrations required for specific processes, in particular by varying frequency, intensity, amplitude, and pressure.

The obtained results provide directions for further research on energy and resource efficiency in the production of classical and NMPCMs for functional purposes.

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